

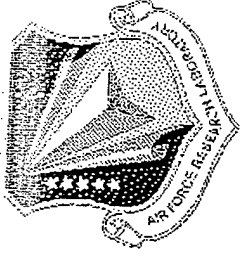
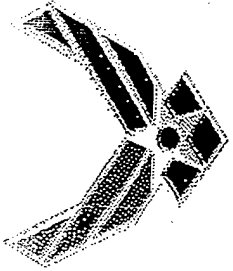
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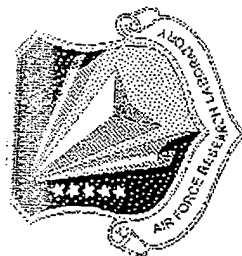
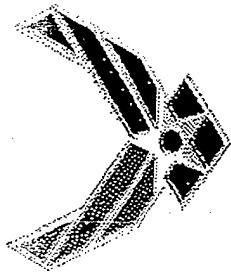
IL QC QSPR - Preliminary Results

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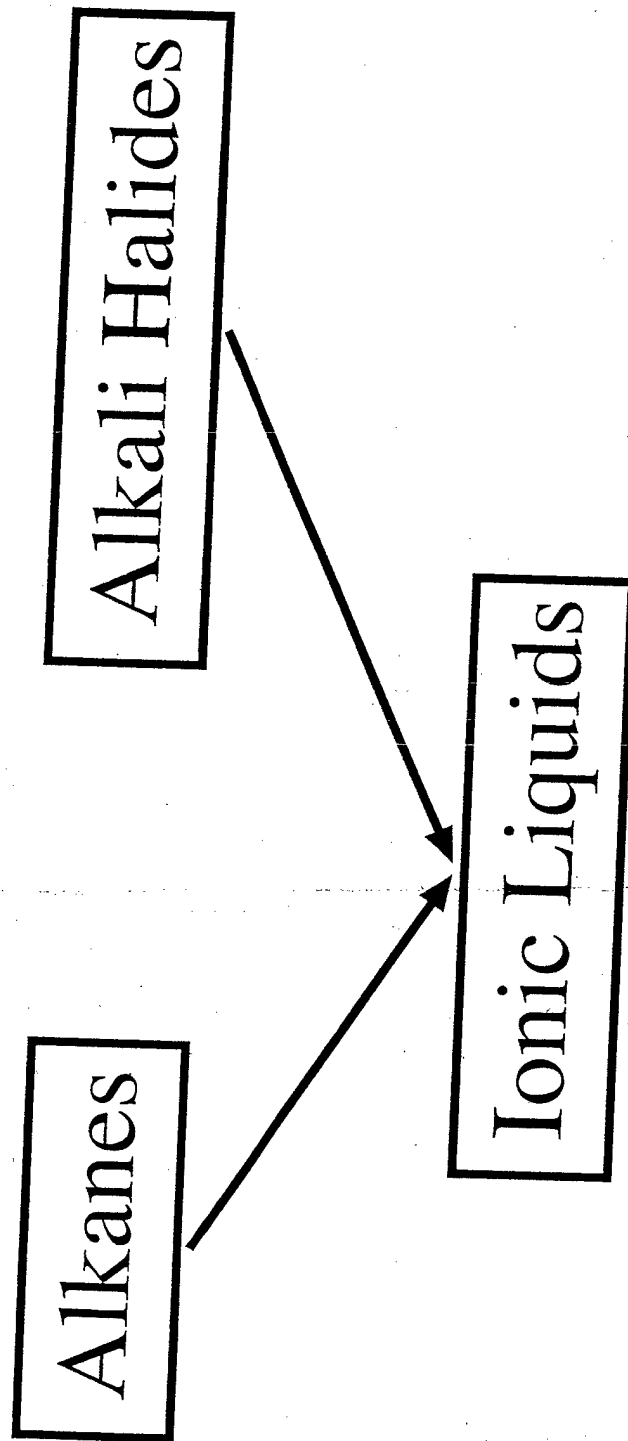
AFRL/PRSP

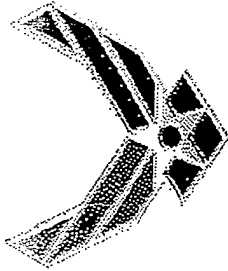
Air Force Research Laboratory
Space and Missile Propulsion Division
Propellants Branch



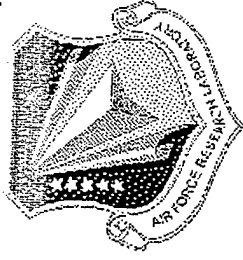
QSPR

Quantitative Structure-Property Relationships Property (Descriptor)





Property (Descriptor)

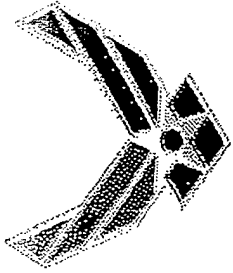


Properties:

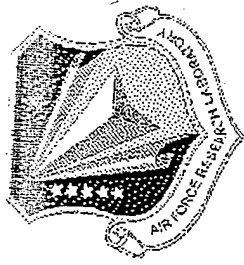
Melting Point
Density (liquid)
(Decomp. Temp.)
(Impact Sensitivity)
(Density (Solid))
(Others ??)

QC Descriptors:

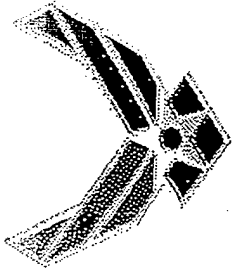
- Single Particle:
Surface Electrostatic
Potential
Surface Size and Shape
- Pair:
Separation
Binding Energy



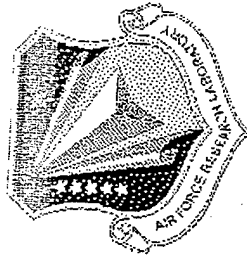
Constraints/Goals



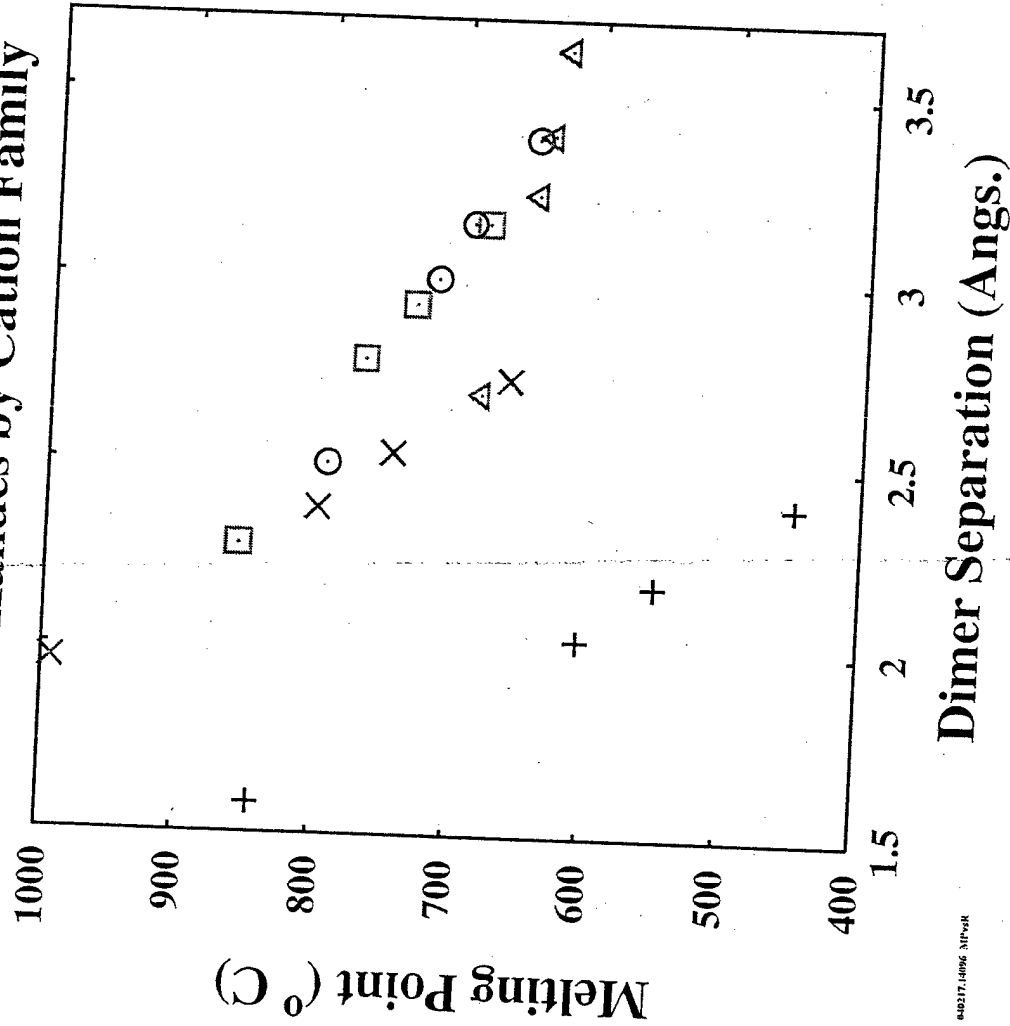
1. Predictive (not just summarize or interpolate)
2. "Universal" Descriptors (Ionic and Nonionic)
3. Allow Ion Interchangability
4. Physically Meaningful and Chemically Ignorant
 - a. No "Kitchen-Sink" Fits
 - b. Charge Symmetry

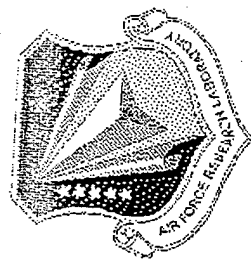
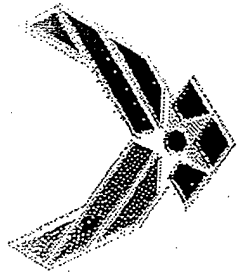


Cation Families Summarized



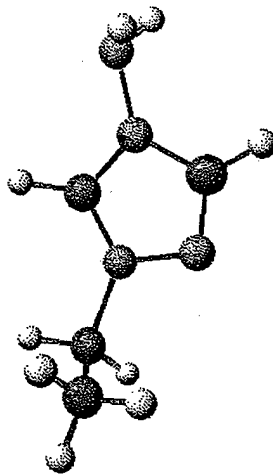
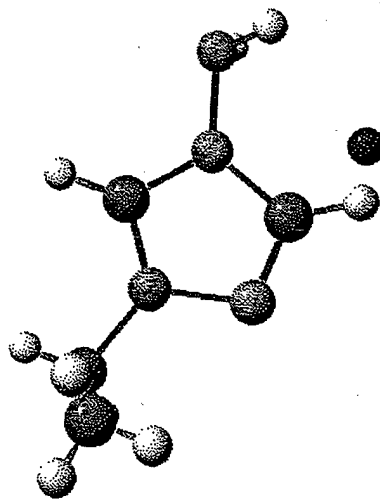
Alkali Halides by Cation Family

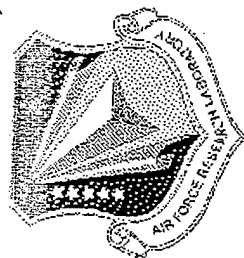
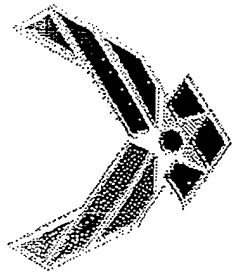




Structures

1-Ethyl-4-amino-1,2,4-triazolium Cation
B3LYP 6-311++G(d,p): Crystal (with Br⁻):





Surface Electrostatic Potential

Color Map:

V at 0.001 au Electron Density:

kcal/mol

350.0

291.7

233.3

175.0

116.7

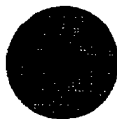
58.3

0.0

Li⁺:



Na⁺:



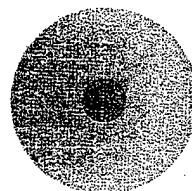
K⁺:

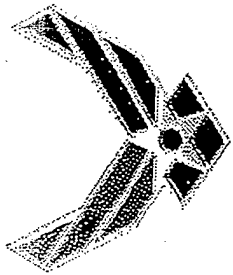


Rb⁺:

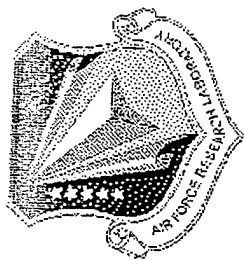


Cs⁺:





Surface Electrostatic Potential

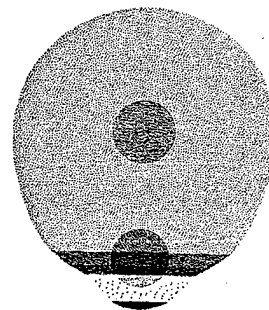
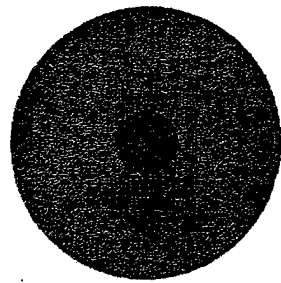
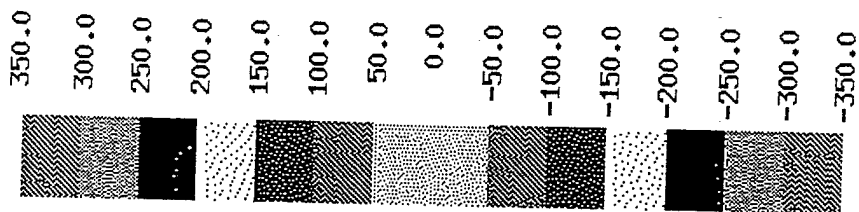


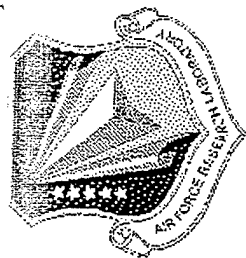
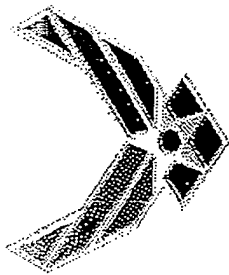
Li^+ :

I^- :

LiI :

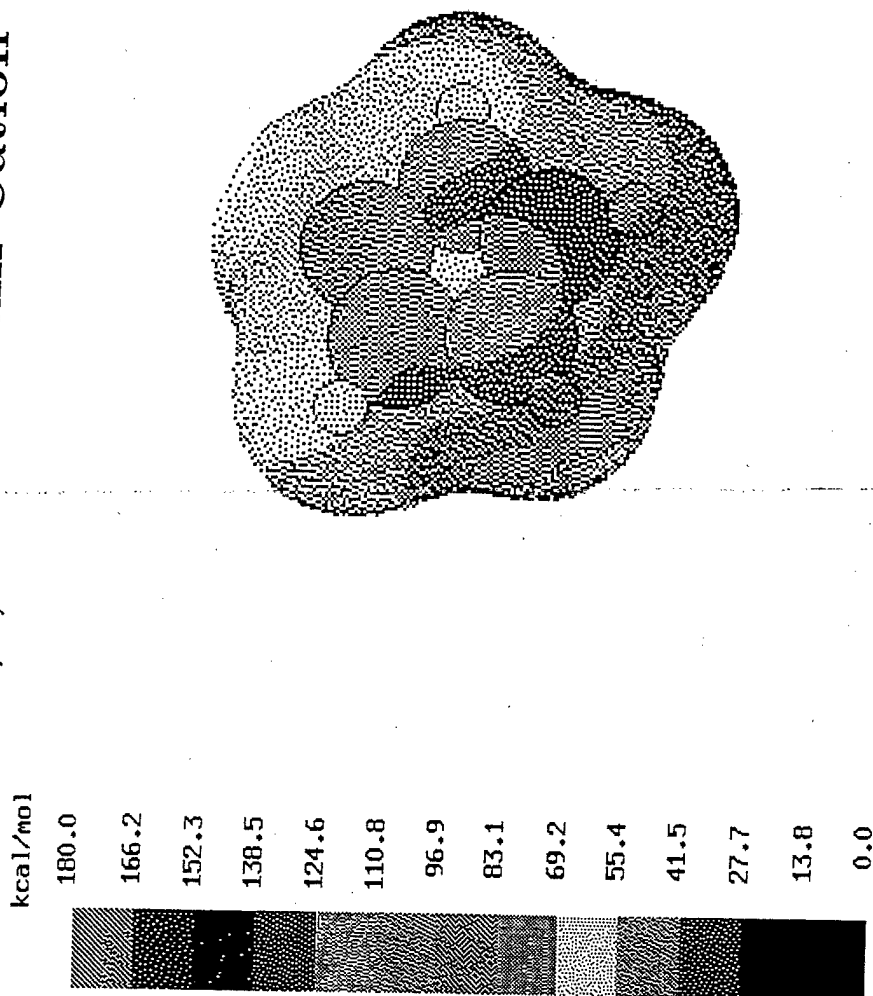
kcal/mol

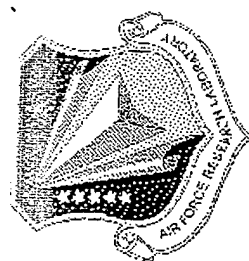




Surface Electrostatic Potential

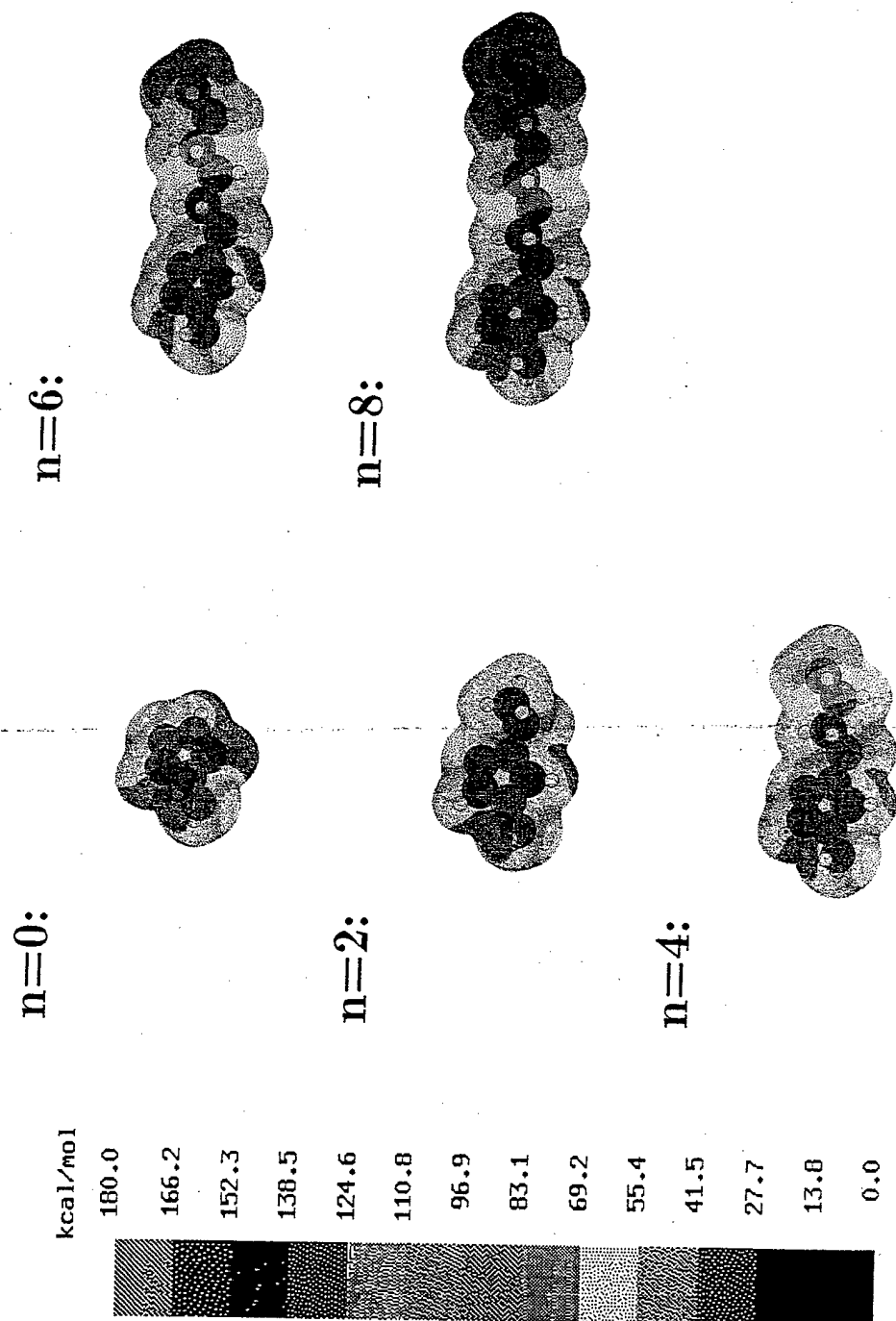
1,2,4-Triazolium Cation

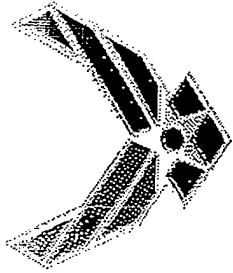




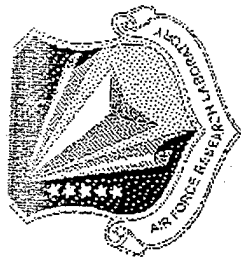
Surface Electrostatic Potential

1-R_n-4-amino-1,2,4-triazolium Cation, n=even:





Descriptors



Electrostatic Potential:

$$\Pi = \frac{1}{A} \sum_i |V_i - \bar{V}| A_i$$

Size:

$$A = \sum_i A_i$$

Shape:

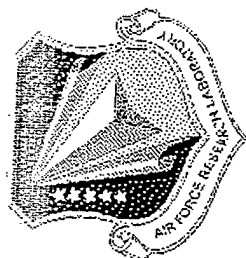
(I_0, I_1, I_2) - PA Moments of Extensia (ordered)

$$\text{Asphericity} = \frac{I_2 - I_0}{I_1}$$

$$\text{Blateness} = \frac{I_1 - I_0}{I_2 - I_0}$$

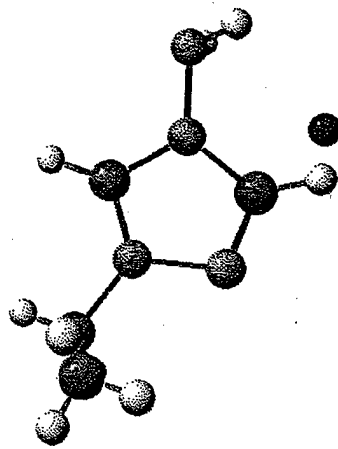


Separation and Interaction Energy



1-Ethyl-4-amino-1,2,4-triazolium Bromide
B3LYP 6-31+G(d):

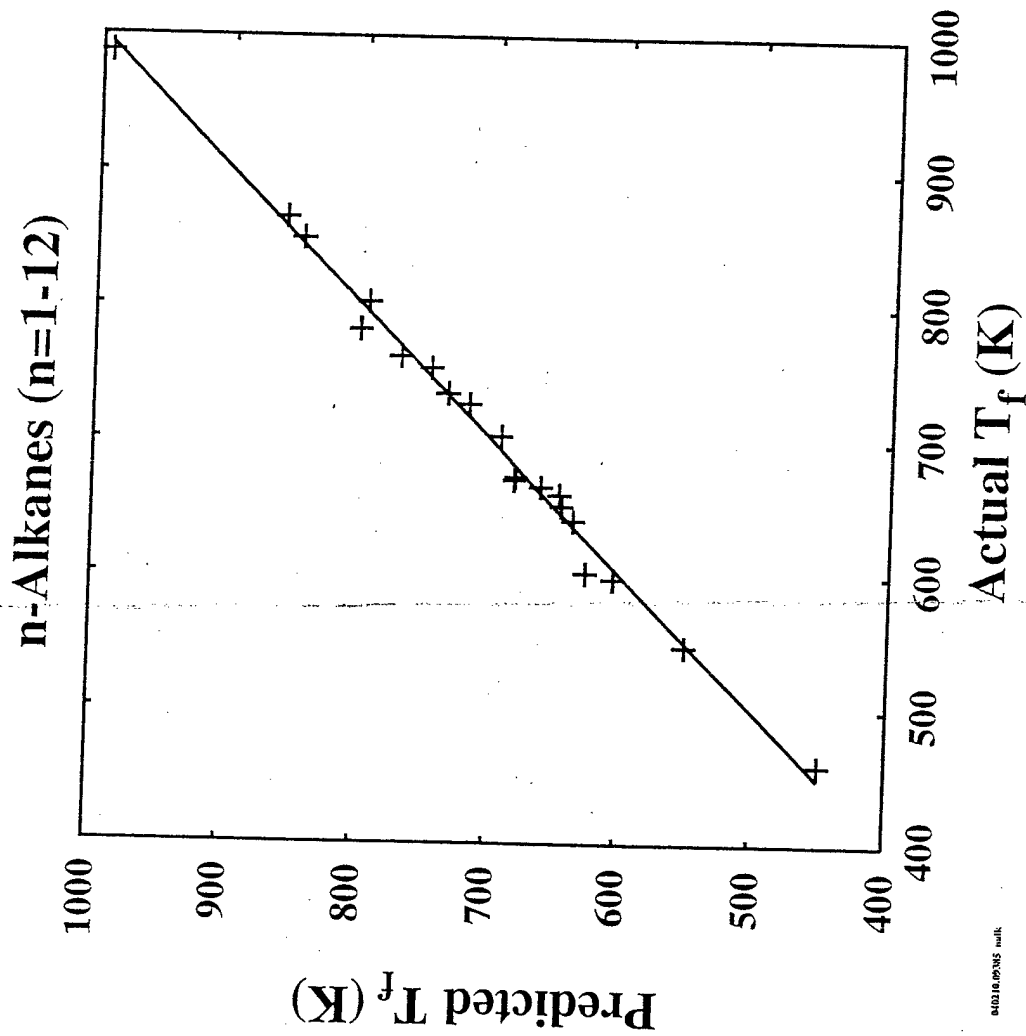
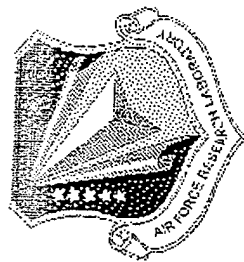
Crystal:



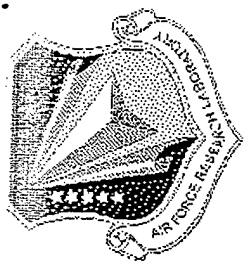
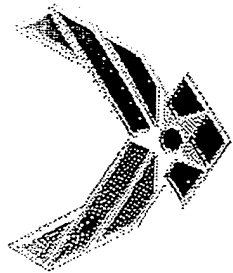
Binding Energy



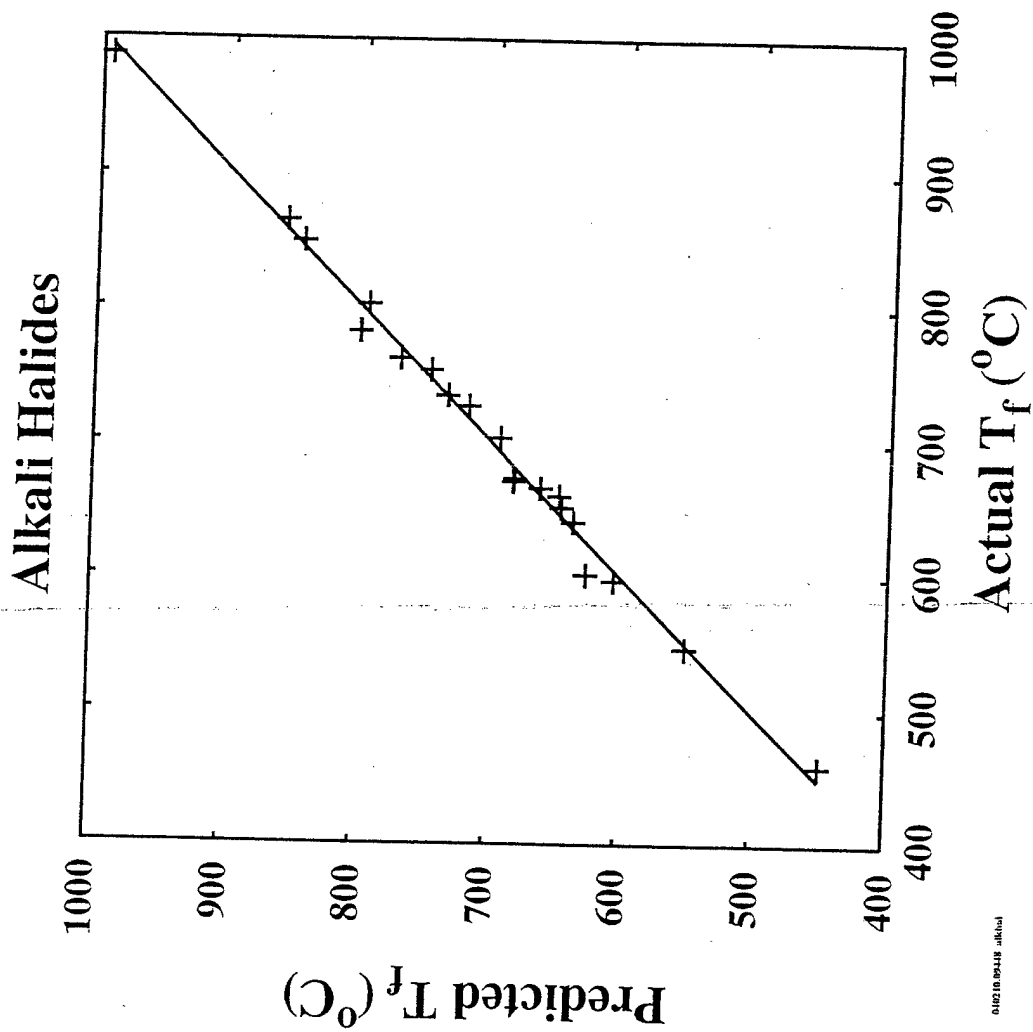
QSPR Correlation



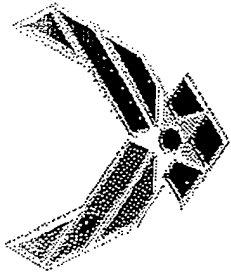
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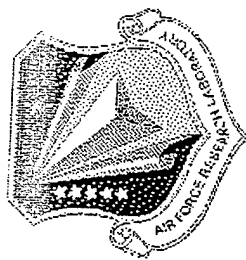
QSPR Correlation



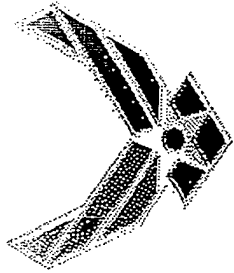
010210 090118 alkhal



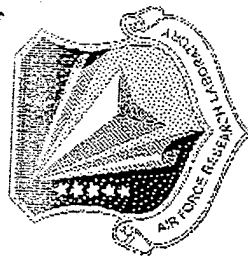
Concluding (Open) Question



Can QC QSPR aid the IL synthesist or will it merely follow?



Acknowledgements



Peter Politzer

J. Boatz

DoD HPCMP - ASC

G. Drake, L. Hall